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Gradient elasto-plasticity with the generalised interpolation material point method

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Abstract

The modelling of geomechanics problems can require a method that allows large deformations and non-linear material behaviour, in this respect the Generalised Material Point Method (GIMPM) is ideal. A fully implicit version of GIMPM has recently been developed for geomechanics problems and some aspects of its implementation are described here. An area that has received less attention in material point methods is that conventional analysis techniques constructed in terms of stress and strain are unable to resolve structural instabilities such as shear banding. This is because they do not contain any measure of the length of the microstructure of the material analysed, such as molecule size or grain structure. Gradient theories provide extensions of the classical equations with additional higher-order terms. The use of length scales makes it possible to model a finite thickness shear band which is not possible with traditional methods. Much work has been done on using gradient theories to include the effect of microstructure in the finite element method (and other numerical analysis techniques) however this yet to be combined with material point methods. In this paper the key equations that are required to extend the implicit GIMPM method to include gradient elasto-plasticity are detailed.

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1. Introduction

The Material Point Method (MPM) suffers from a well documented grid crossing instability [1] when particles cross from one background grid element into another. One method introduced to remedy this is the Generalised Interpolation Material Point method (GIMPM)[2]. The GIMPM modifies particles in the MPM to each have an associated influence domain, the result of this is that there is an increased smoothness of shape functions between elements. This change has been shown to significantly improve the stress response when compared to the MPM [2]. Gradient theories have introduced a length scale through the use of a gradient term as an extension to classical equations. In the literature this has been used for situations including singularities at crack tips, and modelling materials finite thickness shear bands [3]. This paper will be split largely into two sections, first introducing the GIMPM and outlining the difference between the weighting functions used in the GIMPM to the standard shape functions used in the MPM. GIMPM for

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linear elasticity is outlined for the fully implicit approach developed by [4]. The focus of the paper will then switch to elasto-plastic gradient theories, outlining the motivation for wanting to combine gradient elasto-plasticity with the MPM and GIMPM as well as introducing basic elasto-plasticity theory.

2. Implicit GIMPM

The GIMPM was introduced initially by Bardenhagen and Kober [2] as a method to remediate some of the grid crossing errors that exists in the standard MPM. Being consistent with the notation used in the literature the subscript v refers to vertices or grid nodes and p refers to particles or material points. In the GIMPM [2], the standard FEM shape functions are replaced by weighting functions S_{vp} . These functions are constructed from not only on the FEM shape functions, but also a particle characteristic function χ_p specifying the influence of the particle. The weighting function (S_{vp}) can be calculated in a local coordinate system in one dimension (ξ) as

$$S_{vp} = \frac{1}{V_p} \int_{\Omega_p \cap \Omega} \chi_p(\xi) N_v(\xi) d\xi, \quad (1)$$

where V_p is the particle volume (or length in 1D), N_v are the standard linear shape functions with subscript v indicating values are those at grid nodes (or vertices), Ω is the physical domain and Ω_p is the influence domain of the particle. The gradient of the weighting functions (∇S_{vp}), can also be calculated using

$$\nabla S_{vp} = \frac{1}{V_p} \int_{\Omega_p \cap \Omega} \chi_p(\xi) \nabla N_v(\xi) d\xi. \quad (2)$$

The original MPM can be recovered by setting the particle characteristic function equal to the Dirac delta function

$$\chi_p(\xi) = \delta(\xi) V_p. \quad (3)$$

where

$$\delta(\xi) = \begin{cases} 1, & \text{if } \xi = \xi_p \\ 0, & \text{otherwise.} \end{cases} \quad (4)$$

In the GIMPM the use of different functions for $\chi_p(\xi)$ representing a particle's influence domain means that smoother weighting functions can be obtained. The simplest extension is to use a hat function with a value of one within the particle's influence domain, Ω_p , and zero elsewhere. This characteristic function, which is used in the development below can be written as

$$\chi_p(\xi) = \begin{cases} 1, & \text{if } \xi \in \Omega_p \\ 0, & \text{otherwise.} \end{cases} \quad (5)$$

Figure 1 demonstrates graphically how the GIMPM weighting functions can be constructed in one dimension from a convolution of the standard finite element shape functions, N_v , and the particle characteristic function, χ_p , (5). The weighting function at a particular point can be thought of as the integral of the standard shape functions of the associated background grid node over the influence domain of a particle. It can be seen that it is possible that S_{vp} extends outside of the element that the material point is located in.

2.1. Linear Elastic iGIMP method

For a standard linear elastic formulation a linear relationship between stress and strain is assumed

$$\{\sigma\} = [D^e] \{\varepsilon\}, \quad (6)$$

where $\{\sigma\}$ is the Cauchy stress, $[D^e]$ is the elastic stiffness matrix and $\{\varepsilon\}$ is the infinitesimal strain. The strong form statement of equilibrium can be expressed as

$$[L]^T \{\sigma\} = 0, \quad (7)$$

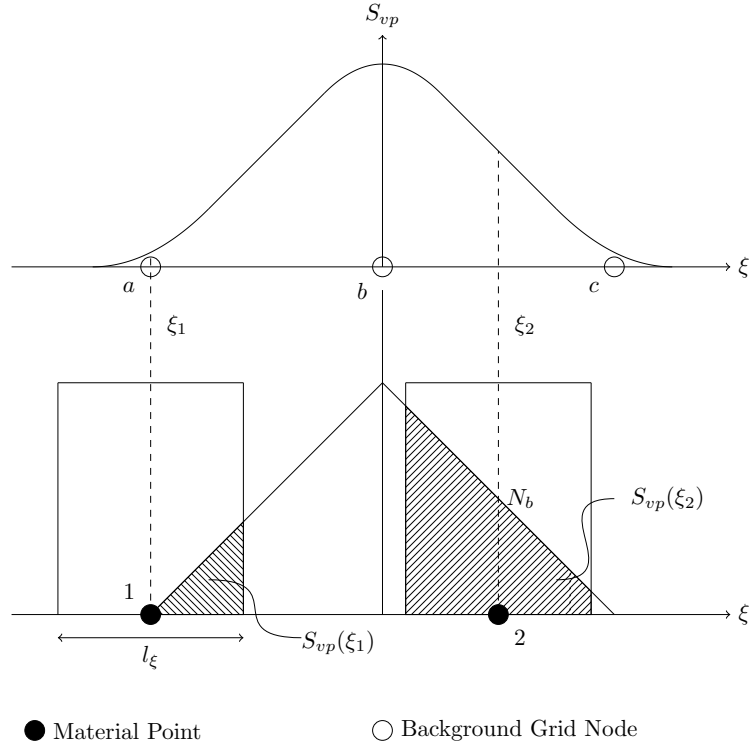


Fig. 1. Weighting function (S_{vp}) at b can be thought of as a convolution of the standard shape function at b (N_b) and a particle's characteristic function χ_p , with width l_ξ .

where $[L]$ is the differential operator matrix. Displacement at a point can be calculated from nodal displacements, $\{d\}$, using the GIMPM shape functions outlined above

$$\{u\} = [S_{vp}]\{d\}. \quad (8)$$

The strain displacement matrix, $[B]$, can be defined as

$$[B] = [L][S_{vp}], \quad (9)$$

given that

$$\{\varepsilon\} = [L]\{u\} \quad (10)$$

it can be shown that

$$\begin{aligned} \{\varepsilon\} &= [L][S_{vp}]\{d\}, \\ &= [B]\{d\}. \end{aligned} \quad (11)$$

From the above definitions it is possible to arrive at the weak form of equilibrium as

$$\int_{\Omega} \{c\}^T [L]^T [D^e] [L] [S_{vp}] \{d\} d\Omega + \int_{\Omega} \{c\}^T \{f_b\} d\Omega = 0, \quad (12)$$

where $\{c\}$ is a test function, $\{f_b\}$ is a body force and Ω is the problem domain. Eliminating the nodal values of the test function, we obtain

$$[K]\{d\} = \{f\}, \quad (13)$$

where $[K]$ is the global stiffness, made up of particle stiffness contributions

$$[K^p] = [B]^T [D^e] [B] v_p. \quad (14)$$

2.2. Implementation

Key differences when implementing GIMPM rather than MPM are the taking into account of the fact that particles can overlap multiple elements. This means that nodes can be effected by not only other nodes in the same element but also those in adjacent elements, increasing the connectivity in the global stiffness matrix. Despite this, GIMP weight functions still possess partition of unity. To create GIMPM shape functions in more than one dimension the tensor product of the one dimensional functions is taken. For full details on the implementation the reader is referred to [4], an outline is given below.

As with the standard MPM, the problem domain is discretised into a set of material points within a regular background grid which extends beyond the physical domain. This is different to FEM as it is necessary for the grid to also cover where material is expected to move into during a simulation. In the GIMPM, influence domains associated with particles are defined to initially cover the the whole of the material with no gaps or overlaps.

At the start of each loadstep the location of each material point with respect to the background grid must be determined, and from this the weighting functions can be computed. Grid elements that do not contain material point domains are also determined and not included in the calculation for this loadstep. At this stage, any external forces on the material points should be incremented and then mapped to the grid nodes. Displacements are calculated using (13) from which stresses are then calculated. At the end of each loadstep, material point positions and domains are updated. The background grid is not updated between loadsteps.

3. Gradient theories

Gradient elasticity theories are an extension of classical elasticity equations to account for microstructure of a material by considering higher order derivatives, these are usually higher order derivatives of displacement or strain. Gradient elasto-plasticity takes the same idea of incorporating higher order derivatives, this time into a elasto-plasticity framework rather than an elastic one and taking derivatives of the plastic multiplier. The phrase 'gradient' comes from these higher order terms being proportional to the Laplacian of lower order terms. An overview of gradient elasticity can be found in [5] by Askes and Aifantis. However, for the types of problem we are interested in modelling, such as shear bands, a gradient elasto-plasticity approach is more appropriate.

3.1. Rate independent elasto-plasticity

Before outlining gradient plasticity it is necessary to first outline the basic concepts of elasto-plasticity theory. Unlike elasticity there is no longer a unique relationship between stress and strain. Initially a yield function f , must be introduced. The yield function is used to define three regions:

- an allowable elastic region inside the yield surface where $f < 0$;
- an inadmissible region outside of the yield surface where $f > 0$; and
- an elasto-plastic boundary on the yield surface where $f = 0$.

That is the stress state must either be on or inside the yield surface. One widely used yield surface is the von Mises yield surface, defined as

$$f = \rho^2 - \rho_y^2 = 0, \quad (15)$$

where ρ_y is the deviatoric yield stress and ρ is the deviatoric stress given by

$$\rho = \sqrt{2J_2} \quad (16)$$

and J_2 is the second stress invariant

$$J_2 = \frac{1}{2} \text{tr}([s][s]). \quad (17)$$

The deviatoric (traceless) stress is $[s] = [\sigma] - I_1[1]/3$, where $[I_1] = \text{tr}([\sigma])$ is the trace of the Cauchy stress $[\sigma]$ and $[1]$ is the three by three identity matrix. In the simplest case, known as perfect plasticity, the yield surface is fixed in

stress space. This will be presented first to highlight the differences needed for gradient elasto-plasticity. It is assumed that the total strain, $\{\varepsilon\}$, can be additively split into an elastic strain, $\{\varepsilon^e\}$, and a plastic strain, $\{\varepsilon^p\}$,

$$\{\varepsilon\} = \{\varepsilon^e\} + \{\varepsilon^p\} \quad (18)$$

and that a rate relationship between exists elastic strain and Cauchy stress

$$\{\dot{\sigma}\} = [D^e]\{\dot{\varepsilon}^e\}, \quad (19)$$

where $[D^e]$ is the linear elastic stiffness matrix. Here we assume an associated plastic flow rule of the form

$$\{\varepsilon^p\} = \dot{\gamma} \left\{ \frac{\partial f}{\partial \sigma} \right\}, \quad (20)$$

where $\dot{\gamma}$ is the plastic consistency parameter controlling the magnitude of plastic strains. The above equations are subject to the the Kuhn-Tucker-Karush consistency conditions

$$\dot{\gamma} \geq 0, \quad f(\{\sigma\}) \leq 0 \quad \text{and} \quad \dot{\gamma} f(\{\sigma\}) = 0. \quad (21)$$

3.2. Gradient elasto-plasticity

Usually in computational plasticity it is necessary to integrate the equations from the previous section to provide an incremental relationship between stress and strain, however in the work here $\dot{\gamma}$ is treated as an independent unknown solved for at nodes in addition to the nodal displacements. The approach described below follows that of De Borst and Mühlhaus [6]. The starting point for this formulation is (12) and (21, part 3) and take into account that, for an incremental value, the elastic strain can be given as the previous elastic strain, plus an increment, minus any increment in plastic straining, that is

$$\{\varepsilon^e\} = \{\varepsilon_n^e\} + \{\Delta\varepsilon\} - \Delta\gamma\{f_{,\sigma}\}, \quad (22)$$

where n refers to the value at the end of the previous loadstep. Taking the weak form of (7) and substituting an incremental relationship for stress gives

$$\int_v \{\delta\varepsilon\}^T [D^e] \{\{\Delta\varepsilon\} - \Delta\gamma\{f_{,\sigma}\}\} dv = - \int_v \{\delta\varepsilon\}^T \{\sigma_n\} dv + \int_s \{\delta u\}^T \{t\} ds \quad (23)$$

where the δ -symbol denotes the variation of a quantity and $\Delta\gamma$ is the increment in the plastic consistency parameter. Taking a Taylor series expansion of the volume averaged version of (21, part 3) it is possible to arrive at

$$\int_v \delta\gamma\{f_{,\sigma}\}^T \{\Delta\sigma\} dv = - \int_v \delta\gamma f(\sigma_n) dv. \quad (24)$$

Using the fact that

$$\{\Delta\sigma\} = [D^e](\{\Delta\varepsilon\} - \Delta\gamma\{f_{,\sigma}\}), \quad (25)$$

it can be written that

$$\int_v \delta\gamma\{f_{,\sigma}\}^T [D^e](\{\Delta\varepsilon\} - \Delta\gamma\{f_{,\sigma}\}) dv = - \int_v \delta\gamma f(\sigma_n) dv. \quad (26)$$

There are now two equations, (23) and (26), in terms of $\{\Delta\gamma\}$ and $\{\Delta\varepsilon\}$. Using the substitutions

$$\Delta\gamma = \{h\}^T \{\Delta\Lambda\} \quad \text{and} \quad \{\Delta\varepsilon\} = [B]\{\Delta d\} \quad (27)$$

where $\{h\}$ are Hermitian shape functions [7] and $[B]$ contains the components of (2). Eliminating $\delta\gamma$ from (26) and substituting $\{\delta\varepsilon\} = [B]\delta c$ and eliminating $\{\delta c\}$ from (23) gives the following equations

$$\int_v [B]^T [D^e] [B] dv \{\Delta d\} - \int_v [B]^T [D^e] \{f_{,\sigma}\} \{h\}^T dv \{\Delta\Lambda\} = \int_s [N]^T dS - \int_v [B]^T \{\sigma_n\} dv \quad (28)$$

and

$$-\int_v \{h\} \{f_{,\sigma}\}^T [D^e] [B] dv \{\Delta d\} + \int_v \{h\} \{f_{,\sigma}\}^T [D^e] \{f_{,\sigma}\} \{h\}^T dv \{\Delta \Lambda\} = \int_v \{h\} f(\sigma_n) dv. \quad (29)$$

which can be re-written as a coupled system

$$\begin{bmatrix} [K_{aa}] & [K_{a\lambda}] \\ [K_{a\lambda}^T] & [K_{\lambda\lambda}] \end{bmatrix} \begin{bmatrix} \{\Delta d\} \\ \{\Delta \Lambda\} \end{bmatrix} = \begin{bmatrix} \int_s [N]^T \{t\} ds - \int_v [B]^T \{\sigma_n\} dv \\ \int_v \{h\} f(\sigma_n) dv \end{bmatrix}, \quad (30)$$

where

$$[K_{aa}] = \int_v [B]^T [D^e] [B] dv, \quad [K_{a\lambda}] = - \int_v [B]^T [D^e] \{f_{,\sigma}\} \{h\}^T dv \quad \text{and} \quad [K_{\lambda\lambda}] = \int_v \{h\} \{f_{,\sigma}\}^T [D^e] \{f_{,\sigma}\} \{h\}^T dv. \quad (31)$$

With this formulation where the plastic consistency parameter is solved alongside displacements it is possible to make the yield strength dependent not only on the plastic strain, but also its Laplacian. To do this, gradient terms must be introduced into the yield function by modifying (15), this means that the yield stress ρ_y used would be replaced with $\rho_y - c \frac{d^2 \epsilon^p}{dx^2}$, for the one dimensional case. $[K_{\lambda\lambda}]$ terms in $[K]$ are also required to be updated as

$$[K_{\lambda\lambda}] = \int_v \{h\} \{f_{,\sigma}\}^T [D^e] \{f_{,\sigma}\} \{h\}^T - c \{h\} \{p\}^T dv. \quad (32)$$

where $\{p\}$ are the laplacians of the Hermitian shape functions and c is a constant that can be related to the material length scale (see [6] for details).

To apply this to the GIMP it should be noted that the Hermitian functions used to map the plastic consistence parameter from the nodes to material points should remain the same. However, the derivatives of shape functions used for mapping the standard strains become the gradient weighting functions outlined earlier in the paper.

4. Conclusions and application to MPM

This paper has, for the first time, described a framework to combine the GIMP with gradient elasto-plasticity to tackle geotechnical problems that contain strain localisation (such as shear banding). The GIMP framework is based on the fully implicit approach of Charlton *et al.* [4] that allows for the analysis of large deformation problems within an updated Lagrangian framework, however for the sake of brevity only the linear version is described in this paper. The elasto-plastic gradient approach of de Borst [6] has been adopted as it provides a straightforward way to implement gradient effects in MPMs (as well as standard rate-independent plasticity). In the approach the plastic consistent parameter becomes an additional nodal unknown that is mapped to the material points using Hermitian shape functions. The use of Hermitian functions are necessary due to the higher-order continuity requirements in gradient theories. In turn, the value of the yield function at the material points becomes an additional error that must be minimised in the coupled non-linear algorithm. The framework can be easily applied to MPMs as all of the equilibrium computations take place on a background finite element grid, making existing finite element technology immediately transferable. The next step is to validate the proposed formulation which will be the focus of a future publication.

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